

1.0 INTRODUCTION

The U.S. Department of Energy (DOE) has committed to prepare a series of Process Model Reports (PMRs) and supporting Analysis Models Reports (AMRs) as the technical bases for the Total System Performance Assessment (TSPA) for the Site Recommendation Consideration Report (SRCR). The purpose of this deliverable is to update the Issue Resolution Status Report (IRSR) of the Evolution of the Near-Field Environment (ENFE). This update reflects the resolution status of the subissue on the effects of coupled thermal-hydrologic-chemical (THC) processes on the waste package chemical environment. The status of resolution is based on a review of the information presented in the PMRs and AMRs. The following AMRs are a subset of those that have been identified in the DOE AMRs/PMRs schedule as relevant to the ENFE subissue on the waste package chemical environment: E0065-AMR on the In-Drift THC Analysis, W0040-AMR on the Pitting and Crevice Corrosion of the Drip Shield in Abstraction Models, and, W0070-AMR on the Surface Environment of the Waste Package and Drip Shield Outer Barrier. The relevant AMRs on features, events, and processes (FEPs) include E0015-FEPs Degradation Modes Analysis, E0110-FEPs EBS Degradation Modes and FEPs Abstraction, N0080-FEPs for the Near-Field Environment, and, WP0055-FEPs for the Waste Package.

Most of the relevant AMRs are unavailable for review at this time. In the following sections, the resolution status description is based on the viability assessment (VA) design and total system performance assessment-viability assessment (TSPA-VA) (U.S. Department of Energy, 1998b). Thus, portions of Section 4.2 from Revision 2 of the ENFE IRSR (U.S. Nuclear Regulatory Commission, 1999c) are preserved. As appropriate, information contained in the license application design selection (LADS) report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999a) and the total system performance assessment (TSPA-SRCR M&A report) (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b) have been used to describe how the approach for the TSPA-SRCR is expected to differ from that of the TSPA-VA (U.S. Department of Energy, 1998b). It is important to note that the TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b) does not contain details on how the different modeling approaches will be implemented. The resolution status of subissue 2 will be further updated as more AMRs and PMRs become available for review.

4.2 EFFECTS OF COUPLED THERMAL-HYDROLOGIC-CHEMICAL PROCESSES ON THE WASTE PACKAGE CHEMICAL ENVIRONMENT

In Revision 2 of its Repository Safety Strategy (U.S. Department of Energy, 1998a), the DOE identified long waste package lifetime as a key factor in its Repository Safety Strategy (U.S. Department of Energy, 1998a). In Revision 3 of the Repository Safety Strategy (U.S. Department of Energy, 2000) the DOE considered performance of the drip shield and performance of the waste package as two of the seven principle factors of the postclosure safety case. Other factors identified by the DOE for the postclosure safety case, though given lower importance, include Environments on the Drip Shield and Environments on the Waste Package.

The model abstraction section of the Yucca Mountain Review Plan (YMRP) is divided into 14 different abstractions. These abstractions are equivalent to the integrated subissues (ISI) in

the Total System Performance Assessment and Integration IRSR (U.S. Nuclear Regulatory Commission, 1999a). The abstractions were referred to as key elements of subsystem abstraction in the flow-down diagram of the ENFE IRSR Revision 2 (U.S. Nuclear Regulatory Commission, 1999c). Waste packages lifetime is embodied in a performance assessment (PA) framework by the ISIs on mechanical disruption of engineered barriers, degradation of engineered barriers, and quantity and chemistry of water contacting waste packages and waste forms (WF). The effects of coupled THC processes only influence the abstraction of the latter two ISIs. Degradation of the engineered barriers, which is addressed explicitly as a subissue in the container life and source-term (CLST) IRSR (U.S. Nuclear Regulatory Commission, 1998), depends strongly on the near-field chemical environment. Performance of the waste packages may also be affected by alternate engineered barrier subsystem design features. As discussed in Section 4.1, the ENFE key technical issue (KTI) will help to evaluate the quantity and chemistry of water contacting the drip shields and waste packages. Contributions from the CLST repository design and thermal-mechanical effects (RDTME), unsaturated and saturated flow under (USFIC), and thermal effects on flow (TEF) KTIs will be required, in addition to contributions from the ENFE KTI, to successfully abstract the two ISIs that are necessary to assess the corrosion of the drip shields and waste packages. DOE must adequately consider coupled THC processes affecting the drip shield and waste package chemical environment in its assessments of repository performance.

4.2.1 Review Methods and Acceptance Criteria

DOE's approach to evaluate and abstract coupled THC processes affecting the waste package chemical environment in a TSPA for the proposed repository at YM is satisfactory if specific acceptance criteria (AC) are met. With this revision (Revision 3) and update of the ENFE IRSR, the AC and review methods (RM) that will be used to evaluate DOE's approach have been moved to the appropriate ISI sections of the YMRP, Revision 0 (U.S. Nuclear Regulatory Commission, 2000a).

4.2.2 Technical Bases for Review Methods and Acceptance Criteria for Effects of Thermal-Hydrologic-Chemical Processes on Waste Package Chemical Environment

The technical bases for the RMs and ACs for coupled THC effects on waste package chemical environment are given in this section. These bases are primarily focused on explaining why the results of coupled THC processes may be important to the drip shield and waste package chemical environment. Limited analyses in past PAs on the effects of coupled geochemical processes on the potential repository waste package environment have been completed. In addition, the relevance to performance of a particular coupled THC process is highly dependent on repository design (e.g., thermal loading strategy and waste package material). This dependence has resulted in AC that primarily focus on ensuring that analyses of the effects are completed. The sophistication of the analysis of the effect of a coupled process on the waste package chemical environment that could be conducted and found acceptable by staff depends on the information available at present, plans to obtain the additional information as part of the long-term testing program, and ability of codes to model coupled processes and determine their impact on repository performance.

Previous versions of the ENFE IRSR (U.S. Nuclear Regulatory Commission, 1999a) reviewed the technical bases for earlier versions of the DOE TSPA analysis of YM. With this revision of the ENFE IRSR, the focus is on updating the technical bases for the RM and AC (see YMRP Revision 0) to reflect the effects of the revised repository design features as they effect the waste package chemical environment through coupled THC processes. The Enhanced Design Alternative II (EDA II) selected as the reference design by DOE during the LADS process (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999a) for TSPA-SRCR calls for a waste package with a corrosion resistant outer barrier, backfill, a titanium (Ti) drip shield, a steel invert with granular ballast, and steel ground support.

4.2.2.1 Coupled Thermal-Hydrologic-Chemical Processes Affecting Waste Package Chemical Environment

The modes and rates of corrosion of container materials are determined by their corrosion potentials in the near-field environment contacting them (Sagar, 1996). The corrosion potential is the potential difference between the container material and a nonpolarizable, reference electrode that is in contact through an electrolyte. The corrosion potential is established by the combination of oxidative and reductive reactions at the container material-solution interface. This potential is an electrochemical parameter that depends on environmental variables, such as temperature, pH, concentration of oxygen, and other reducible species. The potential also is dependent on the composition and surface conditions of the container material. Evaluation of the effects of corrosion potentials on waste package lifetime are treated in detail in the CLST IRSR (U.S. Nuclear Regulatory Commission, 1999b). In the geophysical literature, another potential is noted, called the self-potential or Earth potential. It has been suggested that natural and spontaneous electrical potentials, known as self-potentials, may generate electrical currents that may affect the performance of the waste containers (Wilder, 1996). The components of the self-potential are (see Chapter 8 in Wilder, 1996)

- (1) Streaming potential: This is the potential difference observed due to the pressure differential between two points in the solution/electrolyte phase in continuous contact with a nonconducting solid phase (e.g., rock). The magnitude of the streaming potential decreases with an increase in electrolyte concentration (Newman, 1991) and a decrease in pore radius. In the presence of a conductive solid, the streaming potential decreases through rearrangement of electronic structure within the solid, and a streaming current results.
- (2) Thermoelectric potential: In metallic corrosion literature, thermoelectric potentials are referred to as thermogalvanic potentials. The thermogalvanic potentials consist of thermal diffusion potential (Soret effect) and Nernstian potential due to activity differences at different temperatures.

In contrast to the corrosion potential, the self-potential is established in the electrolyte phase only.

Large self-potentials (greater than 500 mV) have been measured during the single-heater test within the exploratory studies facility (ESF) at YM. The measurements were reported to have been made using the same electrodes that were used for conductivity measurements and were

spaced approximately 1 m apart. Details regarding the input impedance of the voltmeter and the electrode materials are not available at this time. The potential difference, thus, measured above the heater element was about 100 mV and below the heater was about 800 mV. The conductivity measurements indicated that saturation may have increased below the heater. The measured values of self-potentials may be subject to large errors due to (i) the use of polarizable electrodes designed for conductivity measurements, not for self-potential measurements; (ii) the possible use of low-impedance voltmeters that will introduce significant polarization of the electrodes; (iii) the presence of conductive materials; (iv) the discontinuity in the electrolyte layer between measuring points, especially in a variably saturated medium; (v) the contact resistances; and (vi) the lack of filtering of telluric and other sources of noise introduced by the presence of metallic heater elements. These sources of errors have been discussed in geophysical literature (e.g., Corwin and Hoover, 1979) as well as electrochemical literature (e.g., Bard and Faulkner, 1980). For example, assuming the electrode materials were made of platinum typically used in conductivity measurements, the polarization of the electrodes for the oxygen reduction reaction can, by itself, cause a potential difference of over 500 mV (Hoare, 1967). Further information is needed regarding the details of the measurement to assess the accuracy of self-potential measurements made at the ESF. An accurate measurement of self-potentials would entail using nonpolarizable electrodes (e.g., silver/silver chloride or tungsten/tungsten oxide electrodes), high impedance voltmeter (with an input impedance of at least 1 Gigaohm), and signal processing to reduce other sources of noise.

Self-potential is a potential gradient along the solution path, whereas, the corrosion potential is the potential difference across the metal-solution interface. Furthermore, corrosion potentials calculated for container performance explicitly consider the relevant charge transfer reaction equilibrium and kinetics at each spatial location (Mohanty, et al., 1997). Therefore, measured self-potentials should have no effect on waste package performance. If during the performance confirmation period, however, the corrosion potential of the containers is monitored using reference electrodes located at various distances from the container surface, the measured value may be affected by self-potentials. In such a case, an accurate survey of self-potentials at spatial locations relevant to monitoring electrodes should be made. The experimental precautions for accurate measurement of self-potentials mentioned previously apply to this survey.

The ability to calculate moisture redistribution at the drift scale is essential to determine how fast the waste package will corrode. The time period at which the relative humidity (RH) exceeds a critical value, RH_c , is an important factor in determining the container performance. When the RH is less than the RH_c , corrosion of the Ti drip shield and the Alloy 22 waste package will be negligible. Dry oxidation of the engineered barriers may occur, but, the rate of oxidation is expected to be slow for the temperatures specified in the EDA II design. At $RH > RH_c$, corrosion of the Ti drip shield and the Alloy 22 barrier will occur. The type of corrosion and the corrosion rate will depend on the condition of the material (i.e., residual stresses) and the chemistry of the water contacting these engineered barriers. The time at which rewetting of the containers occurs depends on the near-field environment. At this scale, the geometry of the individual waste package becomes important, unlike the repository-scale model in which the waste is assumed to be distributed uniformly. There have been several attempts to model drift-scale moisture distribution (Nitao, 1988; Pruess, Wang, and Tsang, 1990). The problem is difficult because of the variation in scale within the computation domain. Symmetric boundary conditions are usually imposed, implying an infinite array of evenly spaced waste packages.

Thermohydrologic calculation of moisture redistribution is treated specifically in the TEF IRSR (U.S. Nuclear Regulatory Commission, 1998a). Coupled THC effects on moisture redistribution have been noted to induce large effects, such as changes in permeability and porosity (e.g., Hardin, 1998). In general, these effects have been neglected in the thermohydrologic assessments used for YM performance calculations. Also, THC processes will affect the chemistry of gas and water that would interact with the waste package.

Elevated temperatures in the near field at YM are expected to lead to important geochemical changes. In the VA waste package design, oxidation of the carbon steel outer overpack under dry conditions is controlled by the waste package temperature and the composition of the gaseous phase. In particular, the oxygen partial pressure was important for the oxidation of the carbon steel outer barrier. Localized reducing conditions could be promoted by near-field hydrologic effects and phase variations. For the EDA II design, oxidation of the Ti drip shield and the Alloy 22 waste package would be expected to occur at a very slow rate and not result in significant consumption of gaseous species by these engineered barriers. Initial gas flow from the near field, driven by vaporization of water, was predicted to be away from the near field in all directions (Pruess, Wang, and Tsang, 1990; Tsang and Pruess, 1987). This process would tend to purge air containing O_2 and CO_2 from the near-field environment. The vapor pressure of water at temperatures above $95\text{ }^\circ\text{C}$ exceeds the hydrostatic pressure of less than 0.1 MPa at YM. Thus, the gas phase in the near field would tend to be dominated by H_2O under these conditions. Diffusion of air toward zones of relatively high water vapor pressure could reintroduce oxygen to the near field (Tsang and Pruess, 1987). Estimates of the temporal extent of this period of reduced air mass fraction, based on thermal-hydrologic modeling, range from hundreds of years to a few thousand years, depending on thermal loading of the repository (Wilder, 1996; Lichtner, et al., 1997).

Aqueous corrosion of steel sets used as ground support in the repository near field can create a local decrease in Eh, and the corrosion potential. Provided the air mass fraction in the near field remains high, the extent of the reduced zone may be small for various reasons. First, electrochemical reduction of Fe is irreversible (far from equilibrium) and is diffusion-limited in the aqueous phase. Second, corrosion of Fe in an oxidizing environment leads to the formation of Fe oxides and oxyhydroxides that can further decrease the rate of electrochemical reduction of O_2 . Finally, the initial formation of $\alpha\text{-FeOOH}$ can lead to a secondary reduction reaction with Fe_3O_4 . This last process should occur for alternating wet and dry environments (Nishikata, et al., 1994). During the dry period, Fe^{2+} oxides or oxyhydroxides are oxidized by air to $\alpha\text{-FeOOH}$, and the cyclic process proceeds because of the electronic conductivity of the inner layer of Fe_3O_4 .

4.2.2.2 Effects of Waste Package Corrosion Processes on Waste Package Chemical Environment

Corrosion products could have a significant effect on the near-field geochemical environment, which in turn, may affect the nature of ongoing corrosion processes. For example, corrosion of the outer steel overpack of the waste package considered in the TSPA-VA (U.S. Department of Energy, 1998b) might have led to locally reducing conditions in the near field and strong gradients in oxidation potential, despite the prevailing oxidizing nature of the geologic setting (Murphy and Pabalan, 1994). The corrosion rate of the outer steel overpack of the waste package would then adjust to these changes.

Recent changes to the waste package design may reduce the uncertainties associated with the performance of the carbon steel outer overpack specified in the TSPA-VA (U.S. Department of Energy, 1998b). These changes include the elimination of both the carbon steel outer overpack and the concrete lining in the drift. The EDA II repository design specifies steel sets as ground support, a Ti-alloy drip shield, and a corrosion resistant Alloy 22 waste package outer barrier. Geochemical parameters that affect the performance of the steel sets used as ground support via uniform passive or localized corrosion, stress corrosion cracking (SCC), and hydrogen embrittlement include pH, Eh, temperature, Cl^- , NO_3^- , and $\text{HCO}_3^-/\text{CO}_3^{2-}$. For the steel sets used as ground support, alkaline conditions (pH ranging from 8 to 11) provide an environment that results in the formation of a tightly-adhering, passive film, thought to be $\gamma\text{-Fe}_2\text{O}_3$ on carbon steel. This passive film slows down uniform corrosion rates by several orders of magnitude, but makes the metal more prone to the localized breakdown of passivity leading to the occurrence of pitting or crevice corrosion. Should the pH of the water contacting steel sets be neutral (pH = 7) or acidic, then active uniform corrosion will occur. SCC can occur in a $\text{HCO}_3^-/\text{CO}_3^{2-}$ environment at a pH of about 8 when the corrosion potential (related to the Eh of the environment) reaches a critical value.

Corrosion of the drip shields and the waste packages will occur after the formation of water on the surfaces of these engineered barriers as a result of either condensation or dripping. The type of corrosion will be dependent on the chemistry of the water in contact with the metal surfaces. Materials selected for the drip shield (Ti grade 7) and the waste package outer barrier (Alloy 22) are designed to be resistant to localized corrosion. In the absence of localized attack, the degradation of these engineered barriers will occur at a slow rate determined by the passive current density. The localized corrosion of the Ti drip shield and the Alloy 22 waste package outer barrier may result in rapid penetration of the engineered barriers and the possible release of radionuclides. Breakdown of the passive film on Ti grade 7 has been shown dependent on the concentration of fluoride (Brossia and Cragolino, 2000). Localized corrosion of Alloy 22 is possible in oxidizing environments with high chloride concentrations (Dunn, et al., 2000). Elevated chloride and fluoride concentrations have been reported in laboratory tests designed to simulate the effect of evaporation on the chemistry of the environments on the drip shields and waste packages (Gdowski, 1999).

If penetration of the Alloy 22 (or other Ni-base alloys) waste package outer barrier occurs by localized dissolution, further local acidification may result from hydrolysis of Cr^{3+} . Experimental evidence for acidification within crevices of Ni-Cr-Mo alloys has been documented (Cavanaugh, et al., 1983; Sridhar and Dunn, 1994). At higher temperatures, crevice pH lower than one may be found in cracks or pits. It has been shown that the presence of Mo, which is added to increase the corrosion resistance of these alloys, can decrease the pH further, depending on the potential inside the crevice. Increased local acidification and chloride concentration may result in the rapid initiation and penetration of the type 316 NG waste package inner barrier and the subsequent release of radionuclides.

Thus, depending on the rate of movement and dripping of water into the container, the water in immediate contact with the drip shield and the waste package outer barrier may become acidic. Several factors may decrease the corrosion potential established at the drip shield and the waste package outer barrier surface below the repassivation potential for localized corrosion, precluding the occurrence of this phenomenon and, therefore, the generation of acidic conditions.

4.2.2.3 Effects of Cementitious Materials on Waste Package Chemical Environment

Cement is used primarily for its structural (e.g., high compressive strength) and physical (e.g., low permeability) properties. Cements are extremely fine-grained, high-surface area materials containing somewhat soluble and thermodynamically metastable phases that are unstable with respect to crystalline cement phases. These properties and the partially interconnected pore network of the solids make these materials potentially reactive with the near-field environment and the engineered barrier system (EBS).

Cementitious materials may cause changes in near-field chemistry through the time period of regulatory interest, particularly if seepage occurs preferentially along cement-grouted rock bolts. Interactions with cementitious materials will tend to keep $\text{HCO}_3^-/\text{CO}_3^{2-}$ concentrations low. A study by Atkinson, Everitt, and Guppy (1989) indicated that interaction of groundwater typical of a clay environment with cement could maintain a pH above 10.5 for a few hundred thousand years, using the low flow rates assumed in that study. Results of these types of studies are highly dependent on the assumptions used in the calculations, such as groundwater flow rates, amount of cementitious materials present in the repository, and stability of the calcium-silica-hydrate (CSH) gel. Simple extrapolation of results from experiments using laboratory-aged cement pastes is likely to be invalid because the solid and aqueous chemistry of cements will change considerably within the relevant time frame (10–10,000 yrs), even in a closed system (Atkins, Glasser, and Kindness, 1991). For example, Atkinson, Everitt, and Guppy (1989) indicated that, if recrystallization of the CSH gel occurred in the long term, lower pH could result because of the lower solubility of the crystalline CSH phases. Formation of crystalline CSH phases by recrystallization of preexisting CSH gel is likely in a high-level waste (HLW) repository, because of the long time frame involved and the elevated temperatures imposed by radioactive decay heat from emplaced nuclear wastes. Even a modest temperature excursion to 55 °C for 6–12 months can result in partial transformation of the CSH gel to more stable, though poorly crystallized, phases, such as jennite and tobermorite (Atkins, Damidot, and Glasser, 1994). Thus, modeling of cement interactions with the near-field environment and its potential effect on waste package lifetimes must consider the likelihood that cement chemistry is dominated by phases other than those present in the initial material because the dominant phases control the long term evolution of solution pH, a key parameter for container corrosion. Although a number of simulations of the evolution of cement-pore fluid and some simulations of groundwater-cement interactions have been conducted using estimated data (Glasser, Macphee, and Lachowski, 1987; Atkinson, Everitt, and Guppy, 1989; Reardon, 1992; Lichtner and Eikenberg, 1995; Neall, 1996), most of these simulations were conducted for 25 °C and assumed the presence of amorphous CSH gel. Thus, the results may not be relevant to cement-water interactions in a HLW repository.

In the TSPA-VA (U.S. Department of Energy, 1998b) design, the use of cementitious materials, in the form of concrete inverts and linings, was considered for the estimated 179 km of emplacement drifts of the proposed YM HLW repository, in addition to the planned use of cement in roadways for construction and emplacement ramps and service mains. In the TSPA-SRCR design, cementitious materials are not planned for ground support, except in the form of grout to anchor the rock bolts of the ground support system. The potential effect of cementitious materials on the chemical environment for waste package and drip shield corrosion in the TSPA-SRCR design is expected to be substantially reduced compared to the TSPA-VA (U.S. Department of Energy, 1998b) design. However, its effect on the near-field

chemical environment of a repository must be addressed, especially because steel-encased blocks of concrete will be used as invert beneath the waste packages. The degree to which cementitious materials can affect the chemical environment for waste package corrosion will depend to a large part on materials inventory and the reactivity with groundwater of the specific cement material formulation used. Discussion and evaluation of the DOE treatment of concrete/seepage interactions are provided in Sections 5.4.2.2.4 and 5.4.2.3.7.

4.2.2.4 Microbial Effects on Waste Package Chemical Environment

The potential importance of microbial processes to nuclear waste repositories has been recognized internationally for more than 10 yrs, and microbial influenced corrosion of the waste package has been one of the primary concerns (Pedersen and Karlsson, 1995; Stroes-Gascoyne, 1996; Christofi and Philp, 1997). One experiment was explicitly designed to study the gross effects of microbial activity on repository geochemistry, radionuclide sorption, and integrity of repository and host rock materials (West, et al., 1998). This study demonstrated that only localized corrosion of carbon steel could be ascribed to microbial processes. The HLW program has also realized the potential importance of microbial processes on corrosion of waste packages (Geesey, 1993; Horn and Meike, 1995; Civilian Radioactive Waste Management System, Management and Operating Contractor, 1997; TRW Environmental Safety Systems, Inc., 1997). Microbial influenced corrosion is also addressed in the CLST IRSR (U.S. Nuclear Regulatory Commission, 1998a).

The conditions necessary for microbial activity in the near field were discussed in Section 4.1.2.3. Only those aspects that differ and are pertinent to the chemical environment of the waste package are presented here. The amount of nutrients introduced into the repository drifts, which will be potentially available for microbial growth, will be a strong function of both the repository design and the concepts of operation (Wilder, 1996). The potential for microbial growth may be increased greatly if backfill is used. Increased nutrient loading would occur by introduction of the backfill (Stroes-Gascoyne and Gascoyne, 1998; Wilder, 1996). Microbial activity in the tuff system has been demonstrated to be water and organic carbon limited (Kieft, et al., 1997). Thus, if spills of organic fluids are not minimized, then the potential for microbial activity would increase. One additional control on the potential for microbial activity within the emplacement drifts will be temperature and, consequently, the RH (Stroes-Gascoyne, et al., 1996; Civilian Radioactive Waste Management System, Management and Operating Contractor, 1997). For instance, as long as the temperature is above 100 °C or the RH is less than about 60–70 percent, then microbial activity will not occur (Stroes-Gascoyne, 1996; Geesey, 1993). It is likely that the probability of growth of microbes will vary as a function of temperature (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1997).

While microbial activity in the volcanic tuffs will be limited by a lack of nutrients, additional nutrients may be available within the EBS. An analysis of the supply nutrients and energy-producing reactions, which would consume the nutrients, is warranted. Microbial effects on the In-Drift Geochemical Environment (IDGE) will be considered in the TSPA-SRCR. Discussion and evaluation of the DOE treatment of microbial effects are provided in Sections 5.4.2.2.6 and 5.4.2.3.7.

5.4.2 Subissue 2: Effects of Coupled Thermal-Hydrologic-Chemical Processes on the Waste Package Chemical Environment

The YMRP Revision 1 will contain three major chapters for review of the Safety Analysis Report that would accompany a potential license application (LA) for the YM site from the DOE (Lui, et al., 2000). Important topics within the three major chapters will be organized into ISIs. Each ISI has a set of AC and RM. Consequently, the DOE approach in the SR to assess the effects of coupled THC processes on the chemical environment for the waste package chemical environment must meet the following generic AC for each relevant ISI: (i) integration, (ii) data and model justification, (iii) data uncertainty and verification, (iv) model uncertainty; and (v) model verification. Quality assurance is handled in a separate section of the YMRP.

Two model abstraction ISIs are influenced by the ENFE within the scope of the waste package chemical environment subissue: (i) quantity and chemistry of water contacting waste packages and WFs and (ii) degradation of the engineered barriers (U.S. Nuclear Regulatory Commission, 2000a). Both ISIs need to be considered in the evaluation of each DOE abstraction. As part of this evaluation, the AC and RM in the YMRP (U.S. Nuclear Regulatory Commission, 2000a) will be used to review the DOE PMRs and the supporting AMRs as they become available. This evaluation will also include a review of the relevant FEPs included/excluded from the DOE TSPA.

This review focuses on a subset of the AMRs that support the SRCR. These AMRs were chosen to reflect the importance of the abstractions to the DOE safety case and relevance to the ENFE subissue 2. The following AMRs are a subset of those identified in the DOE AMRs/PMRs schedule as relevant to the ENFE subissue 2 on the waste package chemical environment: E0065–AMR on the In-Drift THC Analysis, W0040–AMR on the Pitting and Crevice Corrosion of the Drip Shield in Abstraction Models, and W0070–AMR on the Surface Environment of the Waste Package and Drip Shield Outer Barrier. The relevant AMRs on FEPs include E0015–FEPs Degradation Modes Analysis, E0110–FEPs EBS Degradation Modes and FEPs Abstraction, N0080–FEPs for the Near-Field Environment, and, WP0055–FEPs for the Waste Package.

Only three of the relevant AMRs (E0065, E0015, and W0070) are available for review as of this writing. Staff have not currently completed the review of these AMRs. The resolution status reported here is based on the VA design and TSPA-VA (U.S. Department of Energy, 1998b). As appropriate, status based on information contained in the LADS report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999a) and the TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b) has been included where the approaches differ from those used in the TSPA-VA (U.S. Department of Energy, 1998b). It is important to note that the TSPA-SRCR does not contain details on how the different modeling approaches will be implemented. It is anticipated that the resolution status of subissue will be further updated as more AMRs and PMRs become available for review.

To facilitate the discussion of resolution status on the effects of coupled THC processes on the waste package chemical environment, the AC for the ISIs on (i) quantity and chemistry of water contacting waste packages and waste forms and, (ii) degradation of engineered barriers are listed in Section 5.4.2.1. A summary of the DOE models, abstractions, and analyses relevant to

the waste package chemical environment are presented in Section 5.4.2.2, and staff analyses of the DOE models, abstractions, and analyses are presented in Section 5.4.2.3.

5.4.2.1 Acceptance Criteria

For subissue 2 of the ENFE IRSR, the DOE approach to abstract coupled THC effects on the waste package chemical environment in a TSPA for the proposed repository at YM will be acceptable provided that each AC are met for the ISIs on degradation of the engineered barriers described in Section 4.2.1.3.3.3 of the YMRP, Revision 0 (U.S. Nuclear Regulatory Commission, 2000a) and the quantity and chemistry of water contacting waste packages and waste forms described in Section 4.2.1.3.3.3 of the YMRP, Revision 0 (U.S. Nuclear Regulatory Commission, 2000a). These AC pertain to (i) integration, (ii) data and model justification, (iii) data uncertainty and verification, (iv) model uncertainty, and (v) model verification. A description of these AC taken from the pertinent sections of the YMRP, is given in this section.

Criterion 1: Integration

Integrated Subissue on Quantity and Chemistry of Water Contacting the Waste Packages and Waste Forms

Important design features, physical phenomena and couplings, and consistent and appropriate assumptions have been identified and described sufficiently for incorporation into the abstraction of the quantity and chemistry of water contacting waste packages and WFs in the PA and other related abstractions in the TSPA, and the technical bases are provided. The TSPA abstraction in the DOE LA identifies and describes aspects of the quantity and chemistry of water contacting waste packages and WFs important to waste isolation and also includes the technical bases for these descriptions.

Integrated Subissue on Degradation of Engineered Barriers

Important design features, physical phenomena and couplings, and consistent and appropriate assumptions have been identified and described sufficiently for incorporation into the abstraction of degradation of EBS and other related abstractions in the TSPA, and the technical bases are provided. The TSPA abstraction in the DOE LA identifies and describes design features of the EBS and aspects of the degradation of the EBS important to waste isolation and also includes the technical bases for these descriptions.

Criterion 2: Data and Model Justification

Integrated Subissue on Quantity and Chemistry of Water Contacting the Waste Packages and Waste Forms

Sufficient data on design features (including drip shield, backfill, waste packages, cladding, other EBS components, and thermal loading), geology, hydrology, geochemistry, and geomechanics of the UZ and drift environment (e.g., field, laboratory, and natural analog data) are available to adequately define relevant parameters and conceptual models necessary for developing the abstraction of the quantity and chemistry of water contacting waste packages and WFs in the TSPA. The data are also

sufficient to assess the degree to which FEPs related to the quantity and chemistry of water contacting waste packages and WFs, and which affect compliance with 10 CFR 63.113(b), have been characterized and to determine whether the technical bases provided for inclusion or exclusion of these FEPs are adequate. Where adequate data do not exist, other information sources such as expert elicitation have been appropriately incorporated into the abstraction process.

Integrated Subissue on Degradation of Engineered Barriers

Sufficient data from laboratory corrosion tests and in-service experience in pertinent industrial applications, as well as sufficient site-specific data, including data from drift-scale tests, are available to adequately define relevant parameters and conceptual models necessary for developing the abstraction of the degradation of the EBS in the TSPA. The data are also sufficient to assess the degree to which FEPs related to the degradation of EBS and which affect compliance with 10 CFR 63.113(b) have been characterized and to determine whether the technical bases provided for inclusion or exclusion of these FEPs are adequate.

Criterion 3: Data Uncertainty and Verification

Integrated Subissue on Quantity and Chemistry of Water Contacting the Waste Packages and Waste Forms

Parameter values, assumed ranges, probability distributions, and bounding assumptions used in the TSPA abstraction of quantity and chemistry of water contacting waste packages and WFs, such as pH, chloride concentration, and amount of water flowing in and out of the breached waste package, are consistent with site characterization data, design data, laboratory experiments, field measurements, and natural analog data, are technically defensible, and reasonably account for uncertainties and variabilities. The technical bases for the parameter values used in the TSPA abstraction are provided.

Integrated Subissue on Degradation of Engineered Barriers

Parameter values, assumed ranges, probability distributions, and bounding assumptions used in the TSPA abstraction of degradation of EBS are consistent with data available from laboratory corrosion tests and in-service experiences in pertinent industrial applications, as well as with site-specific data, including data from drift-scale tests, are technically defensible, and reasonably account for uncertainties and variabilities. The technical bases for the parameter values used in the TSPA abstraction are provided.

Criterion 4: Model Uncertainty

Integrated Subissue on Quantity and Chemistry of Water Contacting the Waste Packages and Waste Forms

Alternative modeling approaches consistent with available data (e.g., design features field, laboratory, and natural analog data) and current scientific understanding are investigated and results and limitations are appropriately factored into the abstraction of

quantity and chemistry of water contacting waste packages and WFs. DOE has provided sufficient evidence that ACMs of FEPs have been considered, that the models are consistent with available data and current scientific understanding, and that the effect of these ACMs on the TSPA has been evaluated.

Integrated Subissue on Degradation of Engineered Barriers

Alternative modeling approaches consistent with available data and current scientific understanding are investigated and results and limitations are appropriately factored into the abstraction of the degradation of the EBS. DOE has provided sufficient evidence that ACMs of FEPs have been considered, that the models are consistent with available data (from laboratory corrosion tests and field measurements) and current scientific understanding, and that the effect of these ACMs on the TSPA has been evaluated.

Criterion 5: Model Verification

Integrated Subissue on Quantity and Chemistry of Water Contacting the Waste Packages and Waste Forms

Output from the TSPA abstraction of quantity and chemistry of water contacting waste packages and WFs is justified through comparison with output from detailed process-level models or empirical observations (e.g., laboratory testing, field measurements, and natural analogs).

Integrated Subissue on Degradation of Engineered Barriers

Output from the TSPA abstraction of the degradation of the EBS is justified through comparison with output from detailed process-level models and empirical observations from laboratory tests and field measurements.

5.4.2.2 Description of the U.S. Department of Energy Models, Abstractions, and Analyses

According to the Repository Safety Strategy, principal factors are "central to determining and demonstrating long-term safety of the repository system," and will be the focus of postclosure safety considerations for the SR and LA decisionmaking. Two of the principal factors identified by the DOE for the enhanced repository system are relevant to the ENFE subissue 2: (i) Performance of the Waste Package Barriers and (ii) Performance of Drip Shield. The TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b) outlines how these abstractions will be linked to other abstractions or process-level models in the TSPA-SRCR and the LA to provide the technical basis for the postclosure safety case.

The approach used in the TSPA-VA (U.S. Department of Energy, 1998b) will be modified for the LA and the TSPA-SRCR to refine abstractions and process-level models, take into account the potential effects of the new repository design, and improve coupling between abstractions. Figure 3-1 from the TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b) shows the basic architecture of the new DOE approach. The TSPA-SRCR conceptual model includes five spatial domains that are linked

together by a flow pathway. The spatial domains, sometimes referred to as repository integration process (RIP) cells, are (i) the backfill region above the drip shield; (ii) the drip shield environment, defined as the backfill region immediately on or adjacent to the drip shield; (iii) the waste package environment, defined as the region immediately on, or adjacent to, the waste package (this region include backfill, invert, or corrosion products); (iv) the waste form environment, which includes the interior of the waste package; and (v) the EBS transport pathway environment, which includes the region underneath and between the waste package and drift wall.

Analyses of the two principal factors relevant to ENFE subissue 2 are embodied in the waste package environment cell and in the In-Drift Geochemical submodels that provide input into this cell. The In-Drift Geochemical submodels will be linked to the waste package spatial domain, which acts as a mixing cell, using the new Geochemical Repository Integration Model (GRIM) software. GRIM tracks the seepage flow through each cell and transports the cell's effluent to downstream mixing cells according to prescribed flow paths. Altered solids will remain in each cell for reaction at subsequent times. This approach allows only one-way linkage between subsystem models and TSPA components via output/input transfers at the process model level, or within the TSPA analyses. The EQ3/6 software package (Wolery, 1992) with solid-centered flow through capability will be used to evaluate the In-Drift Geochemistry submodels and to calculate changes to water composition that will be used as input to the waste package cell.

The following six submodels of the DOE In-Drift Geochemical Model described in the TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b) are judged relevant to Subissue 2: Seepage/Backfill Interactions, In-Drift Gas Flux and Composition, In-Drift Microbial Community, Precipitates/Salts Analysis, Corrosion Products, Seepage/Cement Interactions. These submodels are discussed in the following sections. The waste package environment submodels expected to be used to evaluate degradation processes for the TSPA-SR are (i) Humid Air Corrosion, (ii) General Aqueous Corrosion, (iii) Crevice Corrosion, (iv) Pitting Corrosion, (v) SCC, (vi) Hydride Cracking, and (vii) Long-Term Phase Stability.

The following section provides additional information about the individual In-Drift Geochemical and Waste Package Environment submodels relevant to ENFE subissue 2. To highlight the importance of coupled THC processes in the resolution of ENFE subissue 2, discussion of the DOE approach to submodel integration is included as a separate section. Coupled THC processes are not, however, considered a separate DOE abstraction in the TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b). Additional information about the waste package environment submodels is provided in the CLST IRSR (U.S. Nuclear Regulatory Commission, 1998a, 1999b).

5.4.2.2.1 Seepage/Backfill Interactions Submodel

Backfill was not part of the TSPA-VA (U.S. Department of Energy, 1998b) basecase for the near-field geochemical environment (NFGE), but may be included in the EDA II repository design. If backfill is included, and the mineralogy of the backfill materials is different from the host rock, then the water chemistry may change when fluids percolate through the backfill. These changes could affect the performance of the drip shield and the waste package. This submodel will evaluate chemical reactions between water that enters the drift and backfill

materials in the drift to determine the effect on water chemistry. Results will be provided as input to the TSPA Drip Shield Environment and Waste Package Environment models.

5.4.2.2.2 Precipitates/Salts Analysis Submodel

The effects of precipitates/salts on water chemistry were evaluated in near-field sensitivity analyses in support of the TSPA-VA (U.S. Department of Energy, 1998b), but results were primarily used to assess the need for future work in this area. Bounds were placed on the mass and timing of precipitated minerals that might accumulate on the waste package surface, and the capacity for generating highly concentrated brines during the boiling period was evaluated. The progressive evaporation of J-13 water compositions was modeled in two stages, an early stage with <1 molar concentrations and a late stage with >1 molar concentrations. The EQ3/6 Version 7.2b code package was used to evaluate the early evaporative stages. In these calculations, solid solutions were ignored, and the following 12 minerals were suppressed: quartz, K-feldspar, stilbite, mesolite, pyerophyllite, scolecite, muscovite, dolomite, tridymite, clinoptilolite-Ca, albite, and maximum microcline. To simulate late stages of evaporation, simple sets of normative binary salts were constructed to represent the precipitation of the remaining dissolved solids. The types of precipitating salts were primarily chosen based on mass balance and charge balance constraints; however, solubilities reported in the literature also played a role.

The Precipitates/Salts Analysis submodel of the TSPA-SRCR will address more extensive geochemical topics relevant to subissue 2. Calculations will be performed to (i) determine the types and amounts of precipitates (including salts) that might form as a result of evaporation driven by temperature gradients within the drift (e.g., from package surface to drift wall; (ii) explore the effects of progressive evaporation on water chemistry; (iii) evaluate changes to water chemistry as a function of the mass of accumulated precipitates; (iv) determine the effect of time and RH on water vapor condensation; (v) account for back reactions involving the dissolution of precipitates previously deposited on the drip shield, waste package, and other EBS component surfaces; and (vi) predict how much time is required for aqueous species concentrations to return to ambient levels. Results will provide input into the TSPA Drip Shield Environment, Waste Package Environment, and Waste Form Environment models.

5.4.2.2.3 Corrosion Products Submodel

The DOE used process-level models to evaluate the effects of corrosion products in the TSPA-VA (U.S. Department of Energy, 1998b). To support the basecase TSPA-VA (U.S. Department of Energy, 1998b) analyses, the geochemical modeling package EQ3/6 version 7.2b (Wolery, 1992) was used to calculate the composition of water equilibrated with waste package corrosion products of the iron in steel represented by the iron-oxyhydroxide phase goethite (Hardin, et al., 1998, Section 6.4.3.1). Calculations were performed for various stages in the thermal-gaseous evolution of the proposed repository. The initial fluid composition was assumed similar to J-13 well water, except that the total dissolved iron constraint was set to equilibrium with goethite.

In the TSPA-SRCR, the Corrosion Products submodel will evaluate changes to water chemistry due to reactions between metallic components, their corrosion products, and water that percolates into the drift. Metallic components may include the drip shield, the waste packages, the waste package structures, the waste package supports, the rail system, the ground support

systems, and possibly the structural invert materials. The results of these calculations will be provided as input into the TSPA Drip Shield Environment, Waste Package Environment, Waste Form Environment, and Transport Pathway Environment models.

5.4.2.2.4 Seepage/Cement Interactions Submodel

Concrete is a complex solid containing multiple components. The most reactive component of concrete is cement, which itself contains several mineral phases with variable chemical reactivities. The DOE used process-level models to provide input for the effects of seepage/cement interactions in the TSPA-VA sensitivity analyses (U.S. Department of Energy, 1998b). The capacity of the concrete to compete with the CO₂ system for control of the water composition was evaluated for different temperature-gas composition regimes defined by the thermal-hydrology submodel. Local equilibrium was assumed, and changing physical parameters of the concrete (e.g., porosity and density) were not considered. Bounding calculations were performed to increase confidence in the chosen baseline for variables that are highly uncertain from a conceptual or data standpoint. Sensitivity analyses were performed to evaluate the relative reaction rate values for components within the cement mixtures. These analyses were intended to determine the effect of the magnitude of the rate values on the reacted chemistry and to see if the observed dissolution behavior (Berner, 1990) could be recreated by setting all rates to the same value. The effect of suppressed phases on the resultant fluid chemistry was also evaluated.

Calculations for the TSPA-VA (U.S. Department of Energy, 1998b) sensitivity analyses (U.S. Department of Energy, 1998b) were performed using the geochemical modeling package EQ3/6 Version 7.2b (Wolery, 1992). Cement was abstracted as a mixture of SiO₂ and CaH₂SiO₄, or Ca(OH)₂ and CaH₂SiO₄ with log K values dependent on Ca/Si of the solid. To test how the magnitude of the relative reaction rates influenced the reacted fluid chemistry, baseline reaction rate values for all the concrete components were multiplied and divided by five in two separate suites of simulations. This approach assumes that the relative reaction rates for each phase vary independently of each other. A second sensitivity study was performed to test how well the chosen baseline rates recreated the dissolution behavior of cement as outlined by Berner (1990). Reaction rates (rk1) for all components of the concrete were fixed at 1.0 and 0.1 in two separate runs. Changes in the relative reaction rates required that different sized gas reservoirs be available.

At the time of the TSPA-VA (U.S. Department of Energy, 1998b) calculations, it was assumed there would be a concrete liner around the drifts in the proposed repository. A concrete liner is not currently included in the EDA II repository design. Instead, cement is expected only to occur in the form of grout and shotcrete. Hence, the role of concrete in controlling water compositions in the drift may be substantially reduced. The Seepage/Cement interactions submodel of the TSPA-SRCR will evaluate the effects of water/cement reactions on the water chemistry in the drift. The DOE will assume that the cement is initially in equilibrium with the in-drift gaseous phase at the appropriate temperatures. The results of these calculations will be provided as input into the TSPA Backfill, Drip Shield Environment, and Waste Package Environment models.

5.4.2.2.5 In-Drift Gas Flux and Composition Submodel

In the TSPA-VA (U.S. Department of Energy, 1998b), calculations were performed to determine the gas flux and composition in the drift as a function of time and temperature. The results of these calculations provided a framework for beginning additional calculations involving the in-drift geochemical conditions following waste emplacement. Ambient pore gas compositions were input into the thermal-hydrology submodel and allowed to migrate in response to heating. Three different sets of conditions were identified in which the DOE takes the gas composition to be constant: (i) the ambient regime, (ii) the boiling regime, and (iii) the cool-down regime. The geochemical code EQ3/6 Version 7.2b (Wolery, 1992) was used to calculate gas compositions in the last two regimes by equilibrating the fluids in those regimes with the perturbed gas compositions determined in the thermal-hydrological model.

The In-Drift Gas Flux and Composition submodel will evaluate changes in the gaseous phase composition within the repository as a function of time and temperature. Abstractions from the EBS Water Distribution and Removal model and the EBS Physical/Chemical Environment model will be used to set cell-to-cell liquid and gas fluxes within the RIP EBS cell architecture. As a minimum, the In-Drift Gas Flux and Composition submodel will consider the following gas constituents: carbon dioxide, oxygen, nitrogen, and steam. Chemical interactions among the water, gas, and materials in the emplacement drift may act as sources or sinks for constituents in the gas phase. The results of these calculations will be provided as input into the TSPA Backfill, Drip Shield Environment, Waste Package Environment, Waste Form Environment, and Transport Pathway Environment models.

5.4.2.2.6 In-Drift Microbial Communities Submodel

In the TSPA-VA (U.S. Department of Energy, 1998b) technical basis document the DOE included the potential impacts of in-drift microbial communities on the near-field geochemistry as part of their PA of a potential HLW repository at YM. DOE evaluated this topic with the computer code Microbial Impacts to the Near-Field Geochemistry (MING). MING was developed to bound the masses of microorganisms that potentially could be produced in a drift at a potential repository at YM. Following approaches similar to those used in the Canadian HLW repository and the Swiss low/intermediate-level waste repository programs, the DOE computer code uses both mass balance and thermodynamics to quantify the impact of microbial populations. Biomass production is based on both nutrient and energy limitations for microorganisms at YM.

Current work by DOE is focused on bounding the potential abundance of microorganisms in the drift environment based on nutrient and energy limitations. The effects of both thermal loading and introduced materials on microbial abundance will be evaluated as a submodel for the DOE In-Drift Geochemical Model abstraction supporting the TSPA-SRCR (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b).

The Microbial Communities submodel will evaluate nutrient and energy limitations within the drift environment to place bounds on the ultimate abundance of microbes for the TSPA-SRCR. The effects of thermal loading and introduced materials will also be evaluated to predict changes in microbe abundance. The results of these calculations will be provided as input into the TSPA

Drip Shield Environment, Waste Package Environment, Waste Form Environment, and Transport Pathway Environment models.

5.4.2.2.7 Drip Shield and Waste Package Degradation Submodels

The EDA II repository design includes a drip shield made of Ti grade 7 and a waste package with an outer container made of Alloy 22. Although these materials exhibit a high resistance to corrosion, both are susceptible to a variety of localized and general corrosion processes that are influenced by geochemical conditions. The Ti drip shield is expected to develop a protective TiO_2 film on the surface that confers to the metal an extremely high resistance to corrosion in all natural waters, including those with high Cl^- , SO_4^{2-} , PO_4^{2-} , silicate, NO_3^- , and CO_3^{2-} concentrations with a pH range 3–12. Under certain environmental conditions, Ti alloys can be susceptible to crevice corrosion in hot Cl^- solutions (Dunn, et al., 1999). The effects of aggressive environments on the performance of nickel-based alloys, such as Alloy 22, have been studied extensively. Although Alloy 22 is extremely resistant to corrosion as a result of the formation of a Cr-rich oxide film on the metal surface, corrosion rates may increase under certain conditions in solutions with high Cl^- , HS^- , and metastable sulfur oxyanion concentrations (Dunn, et al., 1999). Localized corrosion of Alloy 22 is favored in oxidizing environments with high Cl^- concentrations.

The waste package and drip shield degradation model (WAPDEG) will be integrated with the RIP model in the TSPA-SRCR to allow time-dependent changes in the environment to be considered directly. Seven degradation submodels will be evaluated within the context of the Waste Package Environment RIP cell of the DOE In-Drift Geochemical Model (Figure 3-1). To differentiate between general and localized corrosion processes, the surface of each abstracted drip shield and waste package will be partitioned into discrete regions where degradation processes will be evaluated independently. The submodels expected to be used to evaluate waste package and drip shield degradation processes for the TSPA-SR are (i) Humid Air Corrosion, (ii) General Aqueous Corrosion, (iii) Crevice Corrosion, (iv) Pitting Corrosion, (v) SCC, (vi) Hydride Cracking, and (vii) Long-Term Thermal Stability. Output from these submodels will be in the form of degradation rates and will be used by modules of the WAPDEG (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b) computer code to determine longevity and subsequent degradation areas for the waste package and drip shield.

Environmental parameters required to evaluate the degradation submodels will be supplied by the thermal-hydrology abstraction and the In-Drift Geochemical submodels. The following localized environmental conditions are considered of key importance to the calculation of degradation rates (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b): (i) temperature, (ii) in-drift gases (e.g., H_2O , O_2 , CO_2 , and N_2), (iii) chemistry of water and mineral films on the waste package (e.g., precipitates, salts, and pH), (iv) presence (or absence) of water dripping on the waste package surface, and (v) RH. Time- and temperature-dependent results from the In-Drift Geochemical submodels will be abstracted into lookup tables and then used to constrain the degradation calculations.

The following discussion provides a general description of the drip shield and waste package submodels, indicates which geochemical parameters the submodels are sensitive to, identifies which In-Drift Geochemical submodels will be used to constrain the degradation submodels and

indicates how results from the waste package environment submodels will be abstracted into the TSPA-SRCR. Some of this information is not available currently, and this section will be updated to include new information. Additional information about the degradation submodels may be found in the TSPA-VA (U.S. Department of Energy, 1998b) and the TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b).

5.4.2.2.7.1 Humid Air Corrosion Submodel

In the TSPA-VA (U.S. Department of Energy, 1998b), in which the outer overpack was designed of carbon steel, humid air was assumed to cause active general corrosion of the steel overpack. Humid air corrosion was modeled using a parametric equation exhibiting a dependence of the corrosion rate on time, RH, and absolute temperature. The corrosion rate under humid air conditions was based on abstractions of atmospheric corrosion data from tropical, urban, rural, and industrial locations. The DOE model for humid air corrosion of the VA waste package design was based on the concept of a critical RH. The start of corrosion in a humid air environment was assumed to occur above the critical RH of 65 to 75 percent.

Humid air corrosion may also occur for the Alloy 22 waste package outer barrier proposed in the TSPA-SRCR. The corrosion rates would be lower significantly than those of the carbon steel as a result of the passive behavior of the Ni-base alloy. The method used to abstract the humid air corrosion of the Alloy 22 waste package outer barrier has not been described yet. According to the TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b), future analyses may incorporate the effects of such corrosive environments for different conceptual models of near-field water chemistry, such as those that may result from salt precipitation in a moisture refluxing condition at elevated temperatures.

5.4.2.2.7.2 General Aqueous Corrosion Submodel

The general aqueous corrosion equation used for carbon steel in the TSPA-VA (U.S. Department of Energy, 1998b) did not track geochemical parameters believed to reflect changing environmental conditions in the proposed repository with time. Instead, the dependence of the corrosion rate on time and temperature was obtained from the literature (Boden, 1994; Potter and Mann, 1962) and incorporated into the model development. For example, estimates of the time-dependence of aqueous corrosion were based on long-term corrosion data (up to 16 yrs) in polluted river water (Coburn, 1978) and in tropical lake water (Southwell and Alexander, 1970). These data include the potential effects of microbial activity and various chemical species dissolved in the waters. The General Aqueous Corrosion submodel in the TSPA-VA (U.S. Department of Energy, 1998b) is, therefore, strictly applicable to constant exposure conditions. A "corrosion-time" concept was developed to use the model for time-dependent exposure conditions such as in the potential repository (Lee, Atkin, and Dunlap, 1997). A second critical RH (>85 percent) was used to distinguish the regime of general uniform corrosion in aqueous conditions from humid air corrosion.

The DOE expects Alloy 22 degradation to occur predominantly by general corrosion in the form of passive dissolution (U.S. Department of Energy, 1998b; Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b). General corrosion is normally characterized by a relatively uniform thinning of materials without significant localized

attack that, in the case of corrosion resistant alloys such as Alloy 22, occurs at a low corrosion rate as a result of passivity. General uniform corrosion of the Alloy 22 inner overpack was based on the results of an expert elicitation where the corrosion rate of Alloy 22 was estimated. Two environmental conditions were considered. The first condition corresponds to RHs ranging from 85 to 100 percent in the absence of water dripping. The rates were computed by developing a "composite" distribution using individual expert assessment. The second condition assumed the presence of water dripping onto the waste packages and, therefore, a wide range of local environments. The environmental conditions selected in the expert elicitation were (i) a moderately oxidizing (340 mV versus Standard Hydrogen Electrode) environment with a pH 3–10, (ii) a moderately oxidizing environment with a pH 2.5, and (iii) a highly oxidizing environment (640 mV versus Standard Hydrogen Electrode) environment at a pH 2.5. These environments were assumed to form at localized corrosion sites even though the corrosion itself was considered uniform. The effect of galvanic coupling was ignored, but cladding failure was evaluated as part of this PA.

The abstraction of general corrosion for the Alloy 22 outer barrier proposed for the TSPA-SRCR has not been described. The DOE does not expect that general corrosion of Alloy 22 will lead to a significant number of waste package failures during the first 10,000 yrs after closure. The DOE plans to focus on the most significant mechanisms of engineered barrier degradation, suggesting that the TSPA-SRCR abstraction for the general corrosion of Alloy 22 may be simplified.

5.4.2.2.7.3 Pitting and Crevice Corrosion Submodels

Pitting and crevice corrosion are types of localized corrosion induced by local variations in electrochemical potential on a micro-scale. Localized corrosion may be more sensitive to geochemical conditions than general corrosion. The probability that local corrosion will begin is essentially the probability that an aggressive geochemical environment will exist. In the potential repository environment, such aggressive exposure conditions on the drip shield and waste package would be possible with dripping conditions. The probability of localized corrosion also depends on whether drips are accounted for on the top, sides, or bottom of the waste package and drip shield.

In the TSPA-VA (U.S. Department of Energy, 1998b), crevice corrosion of the Alloy 22 inner barrier was assumed to begin at temperatures greater than or equal to 80 °C with a probability of start equal to zero at 80 °C that increased linearly to one at or above 100 °C. Once started, crevice corrosion was assumed to continue according to a pit growth law. The penetration rate for localized corrosion in the VA was expressed as a function of temperature (T), pH, and the concentrations (C) of NaCl and FeCl₃. Coefficients in the equation were calculated using data for Alloy 22 obtained throughout a broad range of environments that lead to both passive corrosion and localized corrosion. At temperatures less than 80 °C, general corrosion was assumed. Details of the localized corrosion abstractions to be used in the TSPA-SRCR are not available; however, a critical potential to determine the beginning of pitting or crevice corrosion may be used.

5.4.2.2.7.4 Stress Corrosion Cracking Submodel

SCC was not evaluated in the TSPA-VA (U.S. Department of Energy, 1998b). In the TSPA-SRCR, however, the DOE plans to consider SCC of the Alloy 22 outer barrier, particularly in welds. SCC is a failure process characterized by the beginning and propagation of cracks caused by the synergistic interaction of mechanical stress and corrosion reactions. Improper manufacturing can result in preexisting cracks and new cracks may start in areas of high stress concentration, such as at a groove or corrosion pit. Welding residual stress, shrink-fit stress, or weight stress may be sufficient to cause SCC to occur. After a crack begins at specific electrochemical and environmental conditions, the crack will grow when the applied stress intensity factor, K , is equal to or larger than the threshold value of stress intensity for SCC, K_{ISCC} . This process can be represented probabilistically (McCright, 1997). Localized corrosion and SCC are often interrelated because the sites of localized corrosion attack can become the sources of beginning SCC (Farmer and McCright, 1989; Farmer, et al., 1988).

5.4.2.2.7.5 Hydrogen Embrittlement Submodel

Hydrogen embrittlement of Alloy 22 was not evaluated in the TSPA-VA (U.S. Department of Energy, 1998b). The TSPA-SRCR model abstraction will consider hydrogen embrittlement of the Alloy 22 outer barrier. Details of the model abstraction are not presently available.

5.4.2.2.7.6 Long-Term Thermal Stability Submodel

Long-term thermal stability is not evaluated in the TSPA-VA (U.S. Department of Energy, 1998b). The TSPA-SRCR model abstraction will consider long-term thermal stability of the Alloy 22 outer barrier welds. Details of the model abstraction are not presently available.

5.4.2.2.8 Coupling of Thermal-Hydrologic-Chemical Processes

Groundwater composition is sensitive to THC conditions along the flow path, and is expected to evolve as a function of time and space following waste emplacement. For example, the composition of percolating water may change as it interacts with the waste package materials. If thermal loading causes significant evaporation, then secondary precipitates are likely to form on the waste packages causing the composition of the water to change further. These changes in water chemistry are, in turn, likely to affect hydrologic properties along the flow pathway, because porosity and permeability change in response to mineral dissolution and precipitation. The extent of these hydrologic changes is dependent, in part, on the types of phases that precipitate/dissolve, because individual types of phases have characteristic molar volumes. Moreover, the solubilities and precipitation/dissolution rates of the host rock and engineered materials are a function of temperature. Consequently, coupled THC processes affect both ISIs relevant to ENFE subissue 2 and represent an integral part of the DOE conceptual model for PA.

A major assumption of both the TSPA-VA (U.S. Department of Energy, 1998b) and the TSPA-SR is that THC processes can be decoupled, calculated separately, and linked. The basic features of the DOE approach to modeling coupled THC processes in the proposed repository are described in Section 5.4.2.2. As stated in that section, the In-Drift Geochemical submodels will be linked to the waste package spatial domain, which acts as a mixing cell, using the new GRIM software. The TSPA-SRCR M&A report (Civilian Radioactive Waste

Management System, Management and Operating Contractor, 1999b) states that GRIM is expected to provide the following key advantages over the approach used in the TSPA-VA: (i) it facilitates data traceability, data consistency, and output data reproducibility; (ii) it explicitly couples in-drift seepage flux with reaction processes; (iii) it allows assessment of a range of conditions; (iv) it provides time-dependent output of key variables that describe the waste package, waste form, and radionuclide transport environments; and (v) it allows assessment of the effects of coupled chemical processes on drip shield/waste package, and radionuclide transport environments.

5.4.2.3 Analysis of the U.S. Department of Energy Models, Abstractions, and Analyses

Most of the AMRs that provide the details on DOE models, abstractions, and analyses are not available as of this writing. To provide a useful framework for future reviews, the following sections focus on the abstraction architecture described in the Repository Safety Strategy and the TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b). Information provided in the TSPA-VA (U.S. Department of Energy, 1998b) will be considered here only if it is relevant to Subissue 2 and applicable to the handling of abstractions described in the Repository Safety Strategy and TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b).

Staff analysis of DOE models, abstractions, and analyses pertinent to the effects of coupled THC processes on the waste package chemical environment is presented in this section. For this revision of the ENFE IRSR, staff analysis centered on using the AC on integration in reviewing the DOE work. Staff analysis using all five AC will be accomplished as the DOE AMRs and PMRs become available. An analysis of the FEPs relevant to subissue 2 of the ENFE IRSR is presented in the first part of this section, followed by discussions specific to the 13 DOE abstractions.

5.4.2.3.1 Features, Events, and Processes Screening

A formal screening process for FEPs was not developed for the TSPA-VA (U.S. Department of Energy, 1998b), and many important design features, physical phenomena, and couplings were not evaluated in a PA framework. The DOE has since developed a formal documentation of the FEPs identification and screening process in preparation for the TSPA-SRCR. The DOE identification, screening, and documentation process for FEPs is expected to account for known temporal and spatial variations in conditions affecting coupled THC effects on the waste package chemical environment and to relay this information in a thorough and transparent manner.

The contents of the DOE FEPs database (Swift, et al., 1999) have been screened to identify FEPs related to the ENFE subissue 2 on the waste package chemical environment (Pickett and Leslie, 1999; U.S. Nuclear Regulatory Commission, 2000b). The audit review of Pickett and Leslie (1999) indicated that 70 primary FEPs are relevant to ENFE subissue 2 (Table 3-1). Further review of the DOE FEPs database (Swift, et al., 1999) has led to the identification of one additional FEP (2.1.09.02.00—Interaction with corrosion products) that are relevant to the waste package chemical environment subissue. Of the 71 FEPs relevant to subissue 2, 22 were not included by the DOE screening process. In addition, portions of the following three FEPs erre

excluded: FEP 1.1.07.00.00—Repository design, FEP 1.1.08.00.00—Quality control, and FEP 2.1.13.02.00—Radiation damage in waste and EBS. Staff reviewed the 25 FEPs not included and determined that 11 of these should be included. The bases for these determinations are discussed in the following paragraphs. Staff agrees with the DOE disposition for the remaining 60 FEPs identified as relevant to ENFE subissue 2 (Pickett and Leslie, 1999; U.S. Nuclear Regulatory Commission, 2000b), based on screening arguments presented in the FEPs database (Swift, et al., 1999). No further analysis of the relevance of these 60 FEPs to ENFE subissue 2 is anticipated.

Table 3-1 indicates staff judgment on which FEPs are relevant to the DOE abstractions discussed in Section 5.4.2.2. The table shows how DOE abstractions are linked to both DOE included FEPs and DOE excluded FEPs that staff judge to be relevant to ENFE subissue 2. As in Section 5.4.2.2, coupled THC processes are considered a separate DOE abstraction to emphasize their importance to the resolution of ENFE subissue 2. Coupled THC processes are not, however, a separate abstraction in the TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b).

2.1.04.03.00: Erosion or dissolution of backfill

This FEP evaluates the physical and chemical erosion of backfill and was excluded by the DOE. The DOE screening argument for exclusion is that “backfill material at Yucca Mountain will not be highly soluble, and no significant loss due to dissolution is anticipated.” While staff accept that significant erosion of backfill is unlikely, dissolution/precipitation reactions involving backfill and infiltrating waters may lead to significant changes in the composition of the infiltrating waters. The extent of compositional changes to the water would depend, in part, on the composition of backfill selected for the EDA II repository design. After the backfill composition has been established, the DOE should identify and evaluate all water/backfill reactions that may significantly alter the infiltrating water composition. Seepage/Backfill Interactions is one of the DOE In-Drift Geochemical submodels planned for the TSPA-SRCR. Yet, potential effects of seepage/backfill interactions on water composition are not adequately represented in the FEPs database. FEP 2.1.04.05.00 (Backfill Evolution) evaluates the effects of secondary mineralization in backfill on flow. One of these FEPs, either 2.1.04.03.00 or 2.1.04.05.00, should be expanded to include an evaluation on the evolution of water composition through backfill/seepage interactions. As stated in the TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b), changes in water composition through backfill/seepage interactions “may affect drip shield, waste package, and waste form performance”. Results from the Seepage/Backfill Interactions submodel will be provided as input to the TSPA Drip Shield Environment, Waste Package Environment, and Waste Form Degradation models and are relevant to ENFE subissue 2. Any FEP contained within the DOE In-Drift Geochemical submodels also must be contained within the FEPs database.

2.1.06.06.00: Effects and degradation of drip shield

The DOE provided no exclusion/inclusion statement for this FEP, which evaluates the consequences of drip shield degradation by physical and chemical processes. Staff require the inclusion of this FEP because degradation of the drip shield could significantly affect both ISIs encompassed within ENFE subissue 2, Quantity and Chemistry of Water Contacting the Waste

Packages and Waste Forms and Degradation of the Engineered Barriers. Any FEP contained within the DOE In-Drift Geochemical submodels also must be contained within the FEPs database.

2.1.08.07.00: Pathways for unsaturated flow and transport in the waste and engineered barrier system

This FEP evaluates unsaturated flow and radionuclide transport that may occur along preferential pathways in the waste and EBS. The DOE description of this FEP explains that "physical and chemical properties of the EBS and waste form, in both intact and degraded states, should be considered in evaluating pathways." Staff agree with this statement. The DOE screening argument for giving this FEP an "include?" status is too narrowly focused. The screening argument explains that "the details of internal pathways providing release from a container are subsumed in an integrated release distribution." Water compositions are expected to vary depending on the types of materials that the infiltrating waters interact with, and the duration of these interactions. "Chemical properties of the EBS and waste form, in both intact and degraded states" may have a significant influence on flow pathways. This FEP should be included, and its evaluation focused, in part, on potential variations in water composition caused by preferential flow pathways.

2.1.09.02.00: Interaction with corrosion products

The description given for this FEP is "Corrosion products produced during degradation of the metallic portions of the EBS and waste package may affect the mobility of radionuclides. Sorption/desorption and coprecipitation/dissolution processes may occur." Descriptions of associated secondary FEPs cover a broader range of issues. For example, secondary FEP 2.1.09.02.03 (Container Corrosion Products) states that, "Container corrosion products could affect the vault environment, causing significant changes to sorption, transport, dissolution and long-term stability (AECL)". The description of this FEPs requires clarification. Descriptions of primary FEPs should be sufficiently broad to contain the general aspects of related secondary FEPs.

The TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b) describes a submodel called Corrosion Products that will evaluate changes to water chemistry from reactions between metallic components, their corrosion products, and water that percolates into the drift. This submodel is an integral part of the In-Drift Geochemical Model described in the TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b). Any FEP contained with the DOE In-Drift Geochemical submodels also must be contained within the FEPs database. This FEP should be modified to include an evaluation of how water compositions vary as a result of seepage/corrosion product interactions.

2.1.09.07.00: Reaction kinetics in waste and engineered barrier system

The description and screening argument given by the DOE for this FEPs are inconsistent. The FEP description reads, "Chemical reactions, such as radionuclide dissolution/precipitation reactions and reactions controlling the reduction-oxidation state, may not be [in] equilibrium in the drift and waste environment" (U.S. Department of Energy, 1999). The screening argument

only addresses redox reactions. Staff require that DOE clarify the description of this FEP, provide separate screening arguments for redox kinetics, and dissolution/precipitation kinetics, and consider the effects of both types of reaction kinetics under the full range of temperatures expected to exist in the near-field environment during the performance period. According to Section 3.3.4 of the TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b), a major assumption of the DOE IDGE model is that "reactions proceed to equilibrium" because "water movement through the drift is slow compared to the reaction rates between the water and solids in the drift." Staff note that "major assumptions" (U.S. Department of Energy, 1999) are not acceptable as screening arguments for the exclusion of any FEP.

2.1.09.09.00: Electrochemical effects in waste and engineered barrier system

This FEP evaluates electrochemical effects that may establish an electric potential within the drift or between materials in the drift and more distant metallic materials. Ion migration in an electric field could affect corrosion of metals in the EBS and the waste. The DOE excludes this FEP based on the screening argument that "galvanic protection is considered for Yucca Mountain containers." Staff are concerned that electrochemical interactions may alter the chemistry of the water in contact with the waste package and recommend the inclusion of this FEP because of the potential impact these interactions may have on five DOE abstractions related to the waste package environment.

2.1.10.01.00: Biological activity in waste and engineered barrier system

This FEP evaluates biological activity in the waste and EBS that may affect disposal-system performance by altering degradation processes such as waste package and WF corrosion, affecting radionuclide transport through the formation of colloids and biofilms, and generating gases. The DOE category for this FEP was "include?". The TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b) describes a submodel called In-Drift Microbial Communities that will bound the ultimate abundance of microbes and evaluate "changes in microbe abundance due to thermal loading and introduced materials." This FEP addresses FEP related to that submodel, as well as to ENFE subissue 2, and should be included.

2.1.11.08.00: Thermal effects: chemical and microbiological changes in the waste and engineered barrier system

This FEP evaluates how temperature changes in the drift may affect chemical and microbial processes in the waste and EBS. Screening arguments for the exclusion of this FEP were judged inadequate. The rates of near-field processes and microbiological activity may change in response to the thermal pulse generated by waste emplacement. The submodel Microbial Communities will consider "changes in microbe abundance due to thermal loading and introduced materials (TSPA-SRCR M&A)" for the TSPA-SRCR. Any FEP contained within the DOE In-Drift Geochemical submodels also must be contained within the FEPs database. Thus, this FEPs must be included.

2.1.12.01.00: Gas Generation

This FEP evaluates gas generation in the repository by a variety of mechanisms and aggregates these mechanisms into a single category. The DOE screening argument for the exclusion of this FEP is that gas permeability in the repository "is believed to be adequate to allow escape." Staff believe a satisfactory technical basis for determining the inclusion/exclusion status of this FEP should be based on an analysis of the relative rates of gas escape and gas generation. Gas generation could potentially affect the validity of the thermal regimes selected for the TSPA-SR analyses, which will be distinguished from one another, in part, by calculated gas compositions. In addition, exclusion of gas generation processes in the DOE analyses could result in faulty predictions about the abundance and relative proportions of various aqueous species that may be in the drift. Although mass balance calculations performed for the TSPA-VA (U.S. Department of Energy, 1998b) were used to support the assumption that "gas composition is not affected substantially by reaction with the in-drift solids," the DOE must provide sufficient technical bases to demonstrate whether gas generation processes will be significant in the EDA II repository design. Staff conclude the technical basis given for the exclusion of this FEP is inadequate.

2.1.12.05.00: Gas generation from concrete

This FEP evaluates the production of gases from the aging and degradation of concrete that may occur through radiolysis of water in the cement pore spaces and microbial growth on concrete. The screening argument given for the exclusion of this FEP is, "Ignored until importance, if any, can be quantified." In contrast, staff believe that this FEP should be included, until its lack of importance, if any, can be quantified. Concrete may play a smaller role in the TSPA-SRCR than in the TSPA-VA (U.S. Department of Energy, 1998b) because the EDA II repository design is expected to contain a smaller volume of concrete. Moreover, TSPA-VA (U.S. Department of Energy, 1998b) calculations indicate that concrete/seepage interactions would probably not control components of the water and gas composition in the drift. The TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b) includes a Seepage/Cement Interactions submodel that will assess "potential effects of water/cement reactions on chemical conditions in the drift." Staff expect this submodel to include an analysis of gas generation, which is encompassed by FEP 2.1.12.05.00 (Gas Generation from Concrete). Any FEP contained within the DOE In-Drift Geochemical submodels also must be contained within the FEPs database. This FEP should, therefore, be included.

2.1.13.02.00: Radiation damage in waste and engineered barrier system

This FEP evaluates strong radiation fields that "could lead to radiation damage to the waste forms and containers (CSNF, DSNF, DHLW), backfill, drip shield, seals and surrounding rock." Changes to container properties are ignored because they are expected to be small compared to corrosion. Radiation damage to backfill, seals, and rock are excluded because the effects are limited to a distance of about 30 cm from the source. Staff currently do not support the exclusion of radiation damage to container properties, backfill, and seals because adequate screening arguments have not been provided yet.

5.4.2.3.2 Seepage/Backfill Interactions Submodel

Backfill was not part of the TSPA-VA (U.S. Department of Energy, 1998b) basecase for the NFGE and the TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b) does not provide sufficient information to review the DOE approach toward the Seepage/Backfill Interactions submodel. Review of this submodel will occur when the DOE makes the appropriate information available.

Staff note, however, that a key component of the Seepage/Backfill Interactions submodel, as described in the TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b), may not be represented adequately by a FEP. The TSPA-SRCR M&A report indicates that changes in water chemistry owing to seepage/backfill interactions will be evaluated throughout the thermal evolution of the proposed repository. The evolution of water compositions due to backfill interactions is only tangentially covered by secondary FEP 2.1.04.02.09 (Water Chemistry, Tunnel Backfill). This secondary FEP "concerns the chemistry of the water in the tunnel backfill in terms of the concentration of species which influence the longevity of the backfill and the speciation of radionuclides, as well as pH, redox, and chemical gradients, etc." The focus of this FEP appears to be on changes in water chemistry that may influence radionuclide speciation and backfill longevity, and no mention is made of time and temperature dependencies. If backfill is included in the EDA II repository design, then the DOE should clearly define a FEP(s) that adequately captures all the FEPs contained within the Seepage/Backfill Interactions submodel for the TSPA-SRCR.

5.4.2.3.3 Precipitates/Salts Analysis Submodel

The Precipitates/Salts Analysis submodel described in the TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b) addresses a broader range of concerns than the precipitate/salt studies performed in support of the TSPA-VA (U.S. Department of Energy, 1998b). Staff judge the scope of this submodel to be satisfactory in resolving ENFE subissue 2. A detailed review of the DOE approach toward meeting these goals will be performed when the relevant AMRs have been reviewed.

In the TSPA-VA (U.S. Department of Energy, 1998b), the EQ3/6 Version 7.2b code package was used to model the progressive evaporation of J-13 water compositions in two stages, an early evaporative stage with <1 molar concentrations and a late evaporative stage with >1 molar concentrations. The DOE notes that the results of the late stage evaporation analyses have a "high degree of uncertainty" because of a lack of thermodynamic and kinetic data, especially for conditions appropriate for salt formation on the waste package (i.e., high temperature, high ionic strength, and high pH). Attempts were made to compensate for these uncertainties. For example, the DOE ignored solid solutions to increase the concentrations of ions in solution. Overestimating ion concentrations favors waste package corrosion and, therefore, provides a conservative estimate of the effects of precipitates/salts on waste package performance.

Staff do not have confidence that placing bounds on individual parameters will lead to conservative results for the case of concentrated solutions. A large proportion of uncertain parameters are associated with these calculations, and new models are not likely to verify that the results are conservative. As an example, the omission of solid solutions in the TSPA-VA

(U.S. Department of Energy, 1998b) analyses could potentially lead to erroneous predictions about the types and amounts of precipitates that form on the waste package—one of the goals of the Precipitates/Salts submodel described in the TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b). These faulty predictions could, in turn, enhance waste package degradation processes, such as humid air corrosion, or lead to faulty predictions about the chemical composition of the fluids, which then may affect the results of waste form degradation calculations. As stated by the DOE, “sources of solubility data, such as the Handbook of Chemistry and Physics (Weast, 1981), provide mineral solubilities in simple aqueous systems, but they do not provide mineral solubilities for the specific high-pH brines considered here.” The DOE approach toward meeting the goals of the Precipitates/Salts Analysis submodel for the TSPA-SRCR & LA should, therefore, focus on experiments rather than modeling for the case of highly concentrated solutions. Models involving highly concentrated solutions should be developed only where necessary to extrapolate between experiments and to extend the data to relevant conditions not obtainable in the laboratory.

5.4.2.3.4 Corrosion Products Submodel

Corrosion product calculations performed in support of the TSPA-VA (U.S. Department of Energy, 1998b) are not applicable to the EDA II repository design. New data and models are therefore required for the TSPA-SRCR and LA. The DOE must identify the types of corrosion products expected to form on all relevant metallic components in the drift as a function of time and temperature and provide a satisfactory technical basis for these assertions. It must be demonstrated that conservative bounds have been placed on changes in the water chemistry because of corrosion product interactions, especially aqueous species that affect waste package and drip shield degradation processes.

In the TSPA-VA (U.S. Department of Energy, 1998b), goethite was used to represent the corrosion products of the iron in steel (Hardin, et al., 1998), and equilibrium between the incoming water composition and goethite was calculated for each of the DOE time-temperature regimes by forcing the total dissolved iron content to the value required for goethite equilibrium. The DOE specified discrete time-temperature regimes and assumed all reactions proceed to equilibrium within each regime. The major assumption [TSPA-VA (U.S. Department of Energy, 1998b) and the TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b)] that all reactions proceed to equilibrium has not been demonstrated and will not lead to the resolution of ENFE subissue 2 without the introduction of a satisfactory technical basis. Infiltrating waters may react at different rates depending on the type of metallic component involved, and reaction rates are expected to be lower with the introduction of a Ti drip shield and Alloy 22 waste package. Infiltrating waters also may have different residence times on different types of metallic components. For example, percolating water might drip off metallic components, such as railroad ties, but form shallow pools on the ground support systems. The DOE must consider different scenarios to account for potential diversities in both the repository conditions and in the types of metallic components planned in the EDA II repository design. Also, refer to Section 5.4.2.3.9 for discussion of integration.

5.4.2.3.5 Seepage/Cement Interactions Submodel

Although staff generally agree with the approach used to model isolated seepage/cement interactions for the TSPA-VA (U.S. Department of Energy, 1998b), additional consideration must be given to seepage/cement interactions in a complex repository environment. To resolve ENFE subissue 2, which evaluates the effects of *coupled* THC processes on the waste package environment, seepage/cement calculations for the TSPA-SRCR must be expanded to include relevant features in the local environment that may influence the results of this submodel. For example, if concrete is used as a grout material on metal rock bolts, then concrete/metal/seepage interactions should be considered. An acceptable level of approach for this particular case may be, for example, to use water compositions output from the Corrosion Products submodel instead of reacting concrete with the initial infiltrating water composition. DOE calculations on the Seepage/Cement Interactions Submodel for the TSPA-SRCR must be specific to the EDA II repository design and the time-temperature regime being considered.

5.4.2.3.6 In-Drift Gas Flux and Composition Submodel

The In-Drift Gas Flux and Composition submodel for the TSPA-VA (U.S. Department of Energy, 1998b) relied on two assumptions that gas composition is not affected substantially by reaction with the in-drift solids and that a homogeneous gas composition is maintained throughout the in-drift environment. Mass balance calculations were performed to evaluate the first assumption for the TSPA-VA (U.S. Department of Energy, 1998b).

In-drift materials were first assessed for their capacity to act as either sources or sinks of oxygen and carbon dioxide, and then relative masses for the sinks and the sources were compared. The technical basis for this approach will be acceptable for the TSPA-SRCR, but additional mass balance calculations must be performed to determine whether this assumption is also valid for the case of the EDA II repository design. The second assumption involving gas homogeneity was supported by the argument that "gaseous diffusion alone is rapid enough to ensure homogeneity on these scales." Staff accept this argument and do not currently require additional technical bases in support of assumption two.

In the TSPA-VA (U.S. Department of Energy, 1998b), several discrete time regimes were defined to have constant chemical conditions so the description of the NFGE evolution would consist of a set of step changes in system conditions. Temperature and gas compositions were used to define these regimes. If a similar approach is taken for the TSPA-SR, then the DOE must provide a new technical basis for distinguishing between regimes that accounts for new design features and is consistent with results from the In-Drift Gas Flux and Composition Submodel calculations.

Staff support the DOE plans to perform sensitivity studies to learn the effects of different infiltrating water compositions on the in-drift geochemical environment. Technical bases should be provided to explain the DOE position about whether different infiltrating water compositions should or should not be incorporated into repository performance calculations within the context of the In-Drift Geochemical RIP mixing cell architecture TSPA-SRCR M&A report (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b).

5.4.2.3.7 In-Drift Microbial Communities Submodel

In the Final Report TSPA Peer Review Panel (1999), large uncertainties were noted in DOE modeled results because of assumptions made by analysts using MING. Specifically, the report cites DOE efforts to bound microbial growth as a function of biomass production based on nutrient or energy limitations, which require "important, perhaps unknowable, assumptions" (Final Report TSPA Peer Review Panel, 1999). The Panel concluded in the Final Report TSPA Peer Review Panel (1999)

[T]his complex set of assumptions and information requirements used to analyze the contribution of microbial growth leads to a highly uncertain and speculative estimate. Taken as a whole, the Panel does not see the above approach as a clear path to answer the concerns regarding microbial activity. The answers to these questions are not likely to come from more sophisticated models and analysis, which require unavailable information, but rather from bounding analysis and the selection of materials which resist microbial activity.

Staff note the difficulty in placing reasonable bounds on the parameters needed to resolve topics related to microbial activity. Therefore, the clearest path to resolving these concerns at a potential repository at YM is the selection of materials resistant to microbial activity.

5.4.2.3.8 Drip Shield and Waste Package Degradation Submodels

ENFE subissue 2 will not be resolved until staff have determined that results from the In-Drift Geochemical submodels used by the DOE for the TSPA-SRCR and LA will provide sufficient and necessary data to place conservative bounds on geochemical input parameters required to resolve the ISI on Degradation of Engineered Barriers. It is, however, beyond the scope of ENFE subissue 2 to provide an evaluation of the DOE treatment of the drip shield and waste package degradation processes themselves. Detailed reviews of the DOE position on drip shield and waste package degradation processes will be provided in the CLST IRSR Revision 3. Review of the DOE treatment of waste package degradation for the TSPA-VA (U.S. Department of Energy, 1998b) is given in the CLST IRSR Revision 2 (U.S. Nuclear Regulatory Commission, 1999b), Dunn, et al. (1999), and TSPAI IRSR (U.S. Nuclear Regulatory Commission, 1999a).

5.4.2.3.9 Coupled Thermal-Hydrologic-Chemical Processes

The effects of coupled THC processes on seepage and flow were not considered explicitly in the TSPA-VA (U.S. Department of Energy, 1998b). In the ENFE IRSR Revision 2 (U.S. Nuclear Regulatory Commission, 1999c), staff stated

Data and models used in the TSPA-VA (U.S. Department of Energy, 1998b) to calculate the quantity and chemistry of water dripping on waste packages were determined to be inadequate to describe the process and extent of potential dripping under thermally-altered conditions (U.S. Nuclear Regulatory Commission, 1999a). This is an important issue because both DOE and NRC PA analyses indicate that the fraction of waste packages contacted by water is the most important factor affecting dose for the groundwater pathway. In addition,

staff determined that the current DOE testing and modeling plans are not sufficient to resolve the issue prior to LA submission.

The DOE approach for the TSPA-SRCR, like the TSPA-VA will be based on the major assumption that coupled THC processes in the repository environment can be decoupled, considered separately, and then relinked (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b). Given the inherent computational difficulties of evaluating large numbers of coupled processes simultaneously, staff accept the DOE methodology of decoupling/relinking THC processes. Resolution of ENFE subissue 2 will require that the DOE (i) identifies coupled THC processes that may potentially act as important links between individual In-Drift Geochemical submodels, (ii) places reasonable bounds on the affects of coupled THC processes between individual In-Drift Geochemical submodels, and (iii) demonstrates that important coupled THC processes between submodels have been abstracted reasonably into the TSPA-SRCR calculations, and (iv) provides this information in a transparent format.

As an example of how the DOE might accomplish these tasks, consider the TSPA-VA statement that "modeling results of water evaporation indicate that resultant composition may be profoundly affected by the gas phase assumed to be in equilibrium with the evaporating water—i.e., whether the system behaves as open to the atmosphere or in a closed manner (Wilder, 1996; Hardin, et al., 1998, Section 6.2.2)." Murphy and Pabalan (1994) also find that model results are sensitive to the constraints on CO₂ fugacity, with different solid phases precipitating for lower CO₂ fugacities. Predictions about gas compositions and precipitates will be treated in two separate DOE In-Drift Geochemical submodels for the TSPA-SRCR; the In-Drift Gas Flux and Composition submodel and the Precipitates/Salts Analysis submodel. To satisfactorily address the relationship between these two submodels, the DOE might, for example, place bounds on CO₂ fugacities within the context of the In-Drift Gas Flux and Composition submodel and then use these bounds as input into the Precipitates/Salts Analysis submodel. Output from this evaluation, in turn, may be used to constrain the results of additional In-Drift Geochemical submodels, such as the Corrosion Products or Humid Air Corrosion. Staff understand it is impossible to quantitatively evaluate all possible coupled THC processes in this fashion and will accept alternative DOE approaches if demonstrated to be reasonable.

Table 3-1. U.S. Department of Energy (DOE) features, events, and processes (FEPs) database (Revision 00b) (U.S. Department of Energy, 1999) entries relevant to subissue 2 of the Evolution of the Near-Field Environment (ENFE) Key Technical Issue (Pickett and Leslie, 1999). X shows which DOE abstractions are relevant to the FEPs. Numbered columns represent the following DOE abstractions relevant to ENFE subissue 2: (i) Seepage/Backfill Interactions, (ii) Precipitates/Salts Analysis, (iii) Corrosion Products, (iv) Seepage/Cement Interactions, (v) In-Drift Gas Flux and Composition, (vi) Microbial Communities, (vii) Humid Air Corrosion, (viii) General Aqueous Corrosion, (ix) Pitting and Crevice Corrosion, (x) Stress Corrosion Cracking, (xi) Hydride Cracking, (xii) Long-Term Thermal Stability, (xiii) Coupled Thermal-Hydrologic-Chemical Processes.

FEPs Number	FEPs Name	Screening	1	2	3	4	5	6	7	8	9	10	11	12	13
1.1.02.00.00	Excavation/construction	Exclude													
1.1.02.01.00	Site flooding (during construction and operation)	Exclude													
1.1.02.03.00	Undesirable materials remain	Exclude													
1.1.03.01.00	Error in waste or backfill emplacement	Exclude													
1.1.07.00.00	Repository design	Include (exclude deviations from design)	X	X	X	X	X	X	X	X	X	X	X	X	X
1.1.08.00.00	Quality control	Include (exclude defects and deviations)	X	X	X	X	X	X	X	X	X	X	X	X	X
1.1.12.01.00	Accidents and unplanned events during operation	Exclude													
1.1.13.00.00	Retrievability	Include	X	X	X	X	X	X	X	X	X	X	X	X	X
1.2.04.02.00	Igneous activity causes changes to rock properties	Include	X	X	X	X	X	X	X	X	X	X	X	X	X
1.2.06.00.00	Hydrothermal activity	Exclude													
1.2.08.00.00	Diagenesis	Exclude	X	X	X	X	X	X		X	X				X
2.1.01.03.00	Heterogeneity of waste forms	Include	X	X	X	X	X	X	X	X	X	X	X	X	X

Table 3-1. U.S. Department of Energy (DOE) features, events, and processes (FEPs) database (Revision 00b) (U.S. Department of Energy, 1999) entries relevant to subissue 2 of the Evolution of the Near-Field Environment (ENFE) Key Technical Issue (Pickett and Leslie, 1999). X shows which DOE abstractions are relevant to the FEPs. Numbered columns represent the following DOE abstractions relevant to ENFE subissue 2: (i) Seepage/Backfill Interactions, (ii) Precipitates/Salts Analysis, (iii) Corrosion Products, (iv) Seepage/Cement Interactions, (v) In-Drift Gas Flux and Composition, (vi) Microbial Communities, (vii) Humid Air Corrosion, (viii) General Aqueous Corrosion, (ix) Pitting and Crevice Corrosion, (x) Stress Corrosion Cracking, (xi) Hydride Cracking, (xii) Long-Term Thermal Stability, (xiii) Coupled Thermal-Hydrologic-Chemical Processes.

FEPs Number	FEPs Name	Screening	1	2	3	4	5	6	7	8	9	10	11	12	13
2.1.02.01.00	DSNF degradation, alteration, and dissolution	Include	X	X	X			X	X	X	X	X	X	X	X
2.1.02.02.00	CSNF alteration, dissolution, and radionuclide release	Include	X	X	X		X	X	X	X	X	X	X	X	X
2.1.02.03.00	Glass degradation, alteration, and dissolution	Include	X	X	X		X	X		X	X	X	X	X	X
2.1.02.08.00	Pyrophoricity	Exclude													
2.1.03.01.00	Corrosion of waste containers	Include	X	X	X			X		X	X	X	X	X	X
2.1.03.02.00	Stress corrosion cracking of waste containers	Include	X	X	X			X		X	X	X	X	X	X
2.1.03.03.00	Pitting of waste containers	Include	X	X	X			X		X	X	X	X	X	X
2.1.03.04.00	Hydride cracking of waste containers	Include	X	X	X			X		X	X	X	X	X	X
2.1.03.05.00	Microbially-mediated corrosion of waste container	Include	X	X	X			X	X	X	X	X	X	X	X
2.1.03.06.00	Internal corrosion of waste container	Include	X	X	X			X		X	X	X	X	X	X
2.1.03.07.00	Mechanical impact on waste container	Include	X	X	X			X		X	X	X	X	X	X
2.1.03.10.00	Container healing	Include	X	X	X			X		X	X	X	X	X	X

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Table 3-1. U.S. Department of Energy (DOE) features, events, and processes (FEPs) database (Revision 00b) (U.S. Department of Energy, 1999) entries relevant to subissue 2 of the Evolution of the Near-Field Environment (ENFE) Key Technical Issue (Pickett and Leslie, 1999). X shows which DOE abstractions are relevant to the FEPs. Numbered columns represent the following DOE abstractions relevant to ENFE subissue 2: (i) Seepage/Backfill Interactions, (ii) Precipitates/Salts Analysis, (iii) Corrosion Products, (iv) Seepage/Cement Interactions, (v) In-Drift Gas Flux and Composition, (vi) Microbial Communities, (vii) Humid Air Corrosion, (viii) General Aqueous Corrosion, (ix) Pitting and Crevice Corrosion, (x) Stress Corrosion Cracking, (xi) Hydride Cracking, (xii) Long-Term Thermal Stability, (xiii) Coupled Thermal-Hydrologic-Chemical Processes.

FEPs Number	FEPs Name	Screening	1	2	3	4	5	6	7	8	9	10	11	12	13
2.1.03.11.00	Container form	Include	X	X	X		X	X	X	X	X	X	X	X	X
2.1.03.12.00	Container failure (long-term)	Include	X	X	X			X		X	X	X	X	X	X
2.1.04.01.00	Preferential pathways in the backfill	Include	X	X	X			X		X	X	X	X	X	X
2.1.04.02.00	Physical and chemical properties of backfill	Include	X	X	X			X		X	X	X	X	X	X
2.1.04.03.00	Erosion or dissolution of backfill	Exclude	X	X	X			X	X	X	X	X	X		X
2.1.04.05.00	Backfill evolution	Include	X	X	X	X	X	X	X	X	X	X	X	X	X
2.1.06.01.00	Degradation of cementitious materials in drift	Include	X	X	X	X	X	X	X	X	X	X	X	X	X
2.1.06.02.00	Effects of rock reinforcement materials	Include	X	X	X	X	X	X	X	X	X	X	X	X	X
2.1.06.03.00	Degradation of the liner	Include	X	X	X	X	X	X	X	X	X	X	X	X	X
2.1.06.04.00	Flow through the liner	Exclude													
2.1.06.05.00	Degradation of invert and pedestal	Include	X	X	X		X	X	X	X	X	X	X	X	X
2.1.06.06.00	Effects and degradation of drip shield		X	X	X	X	X	X	X	X	X	X	X	X	X

Table 3-1. U.S. Department of Energy (DOE) features, events, and processes (FEPs) database (Revision 00b) (U.S. Department of Energy, 1999) entries relevant to subissue 2 of the Evolution of the Near-Field Environment (ENFE) Key Technical Issue (Pickett and Leslie, 1999). X shows which DOE abstractions are relevant to the FEPs. Numbered columns represent the following DOE abstractions relevant to ENFE subissue 2: (i) Seepage/Backfill Interactions, (ii) Precipitates/Salts Analysis, (iii) Corrosion Products, (iv) Seepage/Cement Interactions, (v) In-Drift Gas Flux and Composition, (vi) Microbial Communities, (vii) Humid Air Corrosion, (viii) General Aqueous Corrosion, (ix) Pitting and Crevice Corrosion, (x) Stress Corrosion Cracking, (xi) Hydride Cracking, (xii) Long-Term Thermal Stability, (xiii) Coupled Thermal-Hydrologic-Chemical Processes.

FEPs Number	FEPs Name	Screening	1	2	3	4	5	6	7	8	9	10	11	12	13
2.1.06.07.00	Effects at material interfaces	Include	X	X	X	X	X	X	X	X	X	X	X	X	X
2.1.08.04.00	Condensation forms on backs of drifts	Include	X	X	X	X	X	X	X	X	X	X	X	X	X
2.1.08.07.00	Pathways for unsaturated flow and transport in the waste and EBS	Include?	X	X	X	X	X	X	X	X	X	X	X	X	X
2.1.08.08.00	Induced hydrological changes in the waste and EBS	Include	X	X	X	X	X	X	X	X	X	X	X	X	X
2.1.08.11.00	Resaturation of repository	Include	X	X	X	X	X	X	X	X	X	X	X	X	X
2.1.09.01.00	Properties of the potential carrier plume in the waste and EBS	Include	X	X	X	X	X	X	X	X	X	X	X	X	X
2.1.09.02.00	Interaction with corrosion products	Exclude?	X	X	X	X	X	X	X	X	X	X	X	X	X
2.1.09.03.00	Volume increase of corrosion products	Exclude	X	X	X		X	X		X	X	X	X	X	X
2.1.09.06.00	Reduction-oxidation potential in waste and EBS	Include	X	X	X	X	X	X	X	X	X	X	X	X	X
2.1.09.07.00	Reaction kinetics in waste and EBS	Exclude	X	X	X	X	X	X	X	X	X	X	X	X	X

Table 3-1. U.S. Department of Energy (DOE) features, events, and processes (FEPs) database (Revision 00b) (U.S. Department of Energy, 1999) entries relevant to subissue 2 of the Evolution of the Near-Field Environment (ENFE) Key Technical Issue (Pickett and Leslie, 1999). X shows which DOE abstractions are relevant to the FEPs. Numbered columns represent the following DOE abstractions relevant to ENFE subissue 2: (i) Seepage/Backfill Interactions, (ii) Precipitates/Salts Analysis, (iii) Corrosion Products, (iv) Seepage/Cement Interactions, (v) In-Drift Gas Flux and Composition, (vi) Microbial Communities, (vii) Humid Air Corrosion, (viii) General Aqueous Corrosion, (ix) Pitting and Crevice Corrosion, (x) Stress Corrosion Cracking, (xi) Hydride Cracking, (xii) Long-Term Thermal Stability, (xiii) Coupled Thermal-Hydrologic-Chemical Processes.

FEPs Number	FEPs Name	Screening	1	2	3	4	5	6	7	8	9	10	11	12	13
2.1.09.08.00	Chemical gradients/enhanced diffusion in waste and EBS	Include	X	X	X			X		X	X	X	X	X	X
2.1.09.09.00	Electrochemical effects (electrophoresis, galvanic coupling) in waste and EBS	Exclude			X					X	X	X	X	X	X
2.1.09.12.00	Rind (altered zone) formation in waste, EBS, and adjacent rock	Include	X	X	X			X		X	X	X	X	X	X
2.1.10.01.00	Biological activity in waste and EBS	Include ?	X		X	X	X	X	X	X	X	X			X
2.1.11.01.00	Heat output/temperature in waste and EBS	Include	X	X	X	X	X	X	X	X	X	X	X	X	X
2.1.11.02.00	Nonuniform heat distribution/edge effects in repository	Include	X	X	X	X	X	X	X	X	X	X	X	X	X
2.1.11.03.00	Exothermic reactions in waste and EBS	Exclude													
2.1.11.04.00	Temperature effects/coupled processes in waste and EBS	Include	X	X	X	X	X	X	X	X	X	X	X	X	X
2.1.11.06.00	Thermal sensitization of waste containers increases fragility	Include	X	X	X			X		X	X	X	X	X	X
2.1.11.08.00	Thermal effects: chemical and microbiological changes in the waste	Exclude	X	X	X	X	X	X		X	X		X		X

Table 3-1. U.S. Department of Energy (DOE) features, events, and processes (FEPs) database (Revision 00b) (U.S. Department of Energy, 1999) entries relevant to subissue 2 of the Evolution of the Near-Field Environment (ENFE) Key Technical Issue (Pickett and Leslie, 1999). X shows which DOE abstractions are relevant to the FEPs. Numbered columns represent the following DOE abstractions relevant to ENFE subissue 2: (i) Seepage/Backfill Interactions, (ii) Precipitates/Salts Analysis, (iii) Corrosion Products, (iv) Seepage/Cement Interactions, (v) In-Drift Gas Flux and Composition, (vi) Microbial Communities, (vii) Humid Air Corrosion, (viii) General Aqueous Corrosion, (ix) Pitting and Crevice Corrosion, (x) Stress Corrosion Cracking, (xi) Hydride Cracking, (xii) Long-Term Thermal Stability, (xiii) Coupled Thermal-Hydrologic-Chemical Processes.

FEPs Number	FEPs Name	Screening	1	2	3	4	5	6	7	8	9	10	11	12	13
	and EBS														
2.1.11.09.00	Thermal effects on liquid or two-phase fluid flow in the waste and EBS	Include	X	X	X			X		X	X	X	X	X	X
2.1.12.01.00	Gas generation	Exclude	X	X	X	X	X	X	X	X	X		X		X
2.1.12.03.00	Gas generation (H ₂) from metal corrosion	Exclude													
2.1.12.04.00	Gas generation (CO ₂ , CH ₄ , H ₂ S) from microbial degradation	Exclude													
2.1.12.05.00	Gas generation from concrete	Exclude	X	X	X	X	X	X	X	X	X		X		X
2.1.12.06.00	Gas transport in waste and EBS	Exclude													
2.1.13.01.00	Radiolysis	Include	X	X	X			X		X	X	X	X	X	X
2.1.13.02.00	Radiation damage in waste and EBS	Include, Exclude (backfill, seals, rock)	X						X	X					
2.2.07.10.00	Condensation zone forms around drifts	Include	X	X	X	X	X	X	X	X	X	X	X	X	X
2.2.07.11.00	Return flow from condensation cap/resaturation of dry-out zone	Include	X	X	X	X	X	X	X	X	X	X	X	X	X
2.2.08.01.00	Groundwater chemistry/composition in UZ and SZ	Include	X	X	X	X	X	X	X	X	X	X	X	X	X

Table 3-1. U.S. Department of Energy (DOE) features, events, and processes (FEPs) database (Revision 00b) (U.S. Department of Energy, 1999) entries relevant to subissue 2 of the Evolution of the Near-Field Environment (ENFE) Key Technical Issue (Pickett and Leslie, 1999). X shows which DOE abstractions are relevant to the FEPs. Numbered columns represent the following DOE abstractions relevant to ENFE subissue 2: (i) Seepage/Backfill Interactions, (ii) Precipitates/Salts Analysis, (iii) Corrosion Products, (iv) Seepage/Cement Interactions, (v) In-Drift Gas Flux and Composition, (vi) Microbial Communities, (vii) Humid Air Corrosion, (viii) General Aqueous Corrosion, (ix) Pitting and Crevice Corrosion, (x) Stress Corrosion Cracking, (xi) Hydride Cracking, (xii) Long-Term Thermal Stability, (xiii) Coupled Thermal-Hydrologic-Chemical Processes.

FEPs Number	FEPs Name	Screening	1	2	3	4	5	6	7	8	9	10	11	12	13
2.2.08.04.00	Redissolution of precipitates directs more corrosive fluids to containers	Exclude	X	X	X	X	X	X	X	X	X	X	X	X	X
2.2.10.01.00	Repository-induced thermal effects in geosphere	Include	X	X	X	X	X	X	X	X	X	X	X	X	X
2.2.11.01.05	Gas generation and gas sources, far-field	Exclude													
2.3.11.03.00	Infiltration and recharge (hydrologic and chemical effects)	Include	X	X	X	X	X	X	X	X	X	X	X	X	X
3.1.01.01.00	Radioactive decay and ingrowth	Include	X	X	X	X	X	X	X	X	X	X	X	X	X

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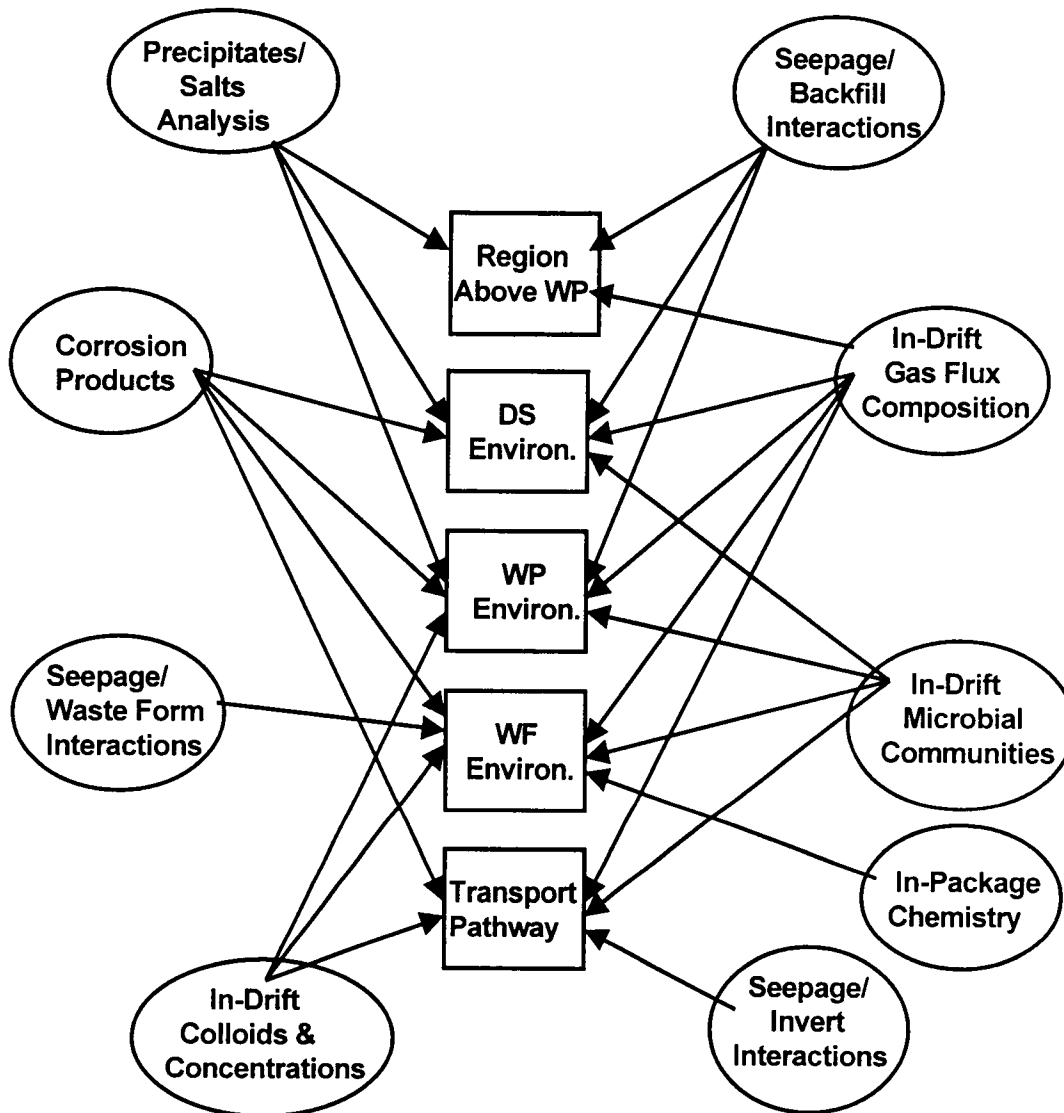


Figure 3-1. DOE's In-Drift Geochemical Model for TSPA-SRCR (Civilian Radioactive Waste Management System, Management and Operating Contractor, 1999b)